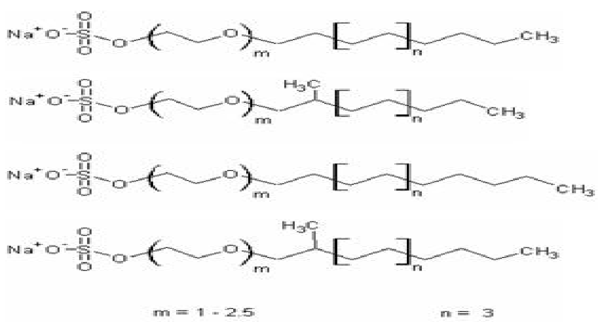
Date: 02/06/2017

Environmental Fact Sheet (#7)

C12-13 E2S Sodium Salt

petrochemical anionic surfactant

Substance Identification			
IUPAC Name	Alcohols, C12-13, branched and linear, ethoxylated, sulphates, sodium salts (1<EO<2.5)	**CAS Number**	161074-79-9
Other Names	Alcohol C12-13 ethoxysulfate		
Molecular Formula	UVCB substance (substances of Unknown or Variable composition, Complex reaction products or Biological materials), no univocal molecular formula available	Structural formula: 	

Physical/Chemical Properties [1]	
Molecular Weight	376.48-390.51 g/mol
Physical state	Solid
Appearance	Yellow paste
Density	1.08 at 22°C (Approach: read-across based on grouping of substances)
Melting Points	ca. 188 °C at 101.8 kPa
Boiling point	192.68 °C at 101.8 kPa
Flash Point	Study technically not feasible (irrelevant property for solids)
Vapour Pressure	< 5Pa at 20-50°C
Water Solubility	280 g/l at 20°C (Approach: read-across based on grouping of substances)
Flammability	Solid: flammable (Approach: read-across based on grouping of substances)
Explosive Properties	No data available
Surface Tension	28.24 mN/m at 25 °C
Octanol/water Partition coefficient (Kow)	log K_{OW} = 1.5 at 20 °C
Product and Process Description	C12-13 E2S is an anionic surfactant of petrochemical origin. It belongs to the group of alcohol ethoxy sulphates (AES). The Alcohol ethoxy sulphates, also known as alcohol ether sulphates, are derived from petro- or oleochemical alcohols. They are manufactured by the sulphation of alcohol ethoxylates, generally containing 1-4 ethylene oxide units [6]. Sodium salts of AES are by far the commonly used grades. Four steps are involved in the manufacture of AES: alcohol production, ethoxylation, sulphation and neutralization. C12-13 E2S (petro) is manufactured by the reaction of the ethoxylate of fatty alcohol from

	petrochemical sources, with sulphur trioxide in a falling film reactor. In these reactors, a thin film of material to be sulphated flows down the inside surface of vertical tubes through which dry air containing SO3 is passed. The reaction takes place at the gas-liquid interface with a degree of conversion in excess of 98%. The heat of reaction is removed by a cooling agent flowing around the outside of the tubes and may be subsequently recovered. The resulting acid is immediately neutralized, typically with sodium hydroxide, ammonia or ethanol amines. Here the production of the most common product, the sodium salt, is considered [5].
Application	AES are used by the personal care, household, agriculture, oilfield, mining, coatings and lubricant industries. Their properties make them particularly well-suited for use in shampoos, bath and shower products, body cleansing products, manual dish detergents, etc.

Life Cycle Assessment

General Introduction

These Environmental Fact Sheets are a product of the *ERASM Surfactant Life Cycle & Ecofootprinting (SLE)* project. The objective of this project was to establish or update the current environmental profile of 15 surfactants and 17 precursors, taking into consideration actual surfactant production technology and consistent high quality background data.

The Fact Sheets are based upon life cycle assessment (LCA) and have been prepared in accordance with the ISO standard [ISO 14040: 2006 and ISO 14044: 2006]. In addition, the project follows the ILCD (2010) handbook. This fact sheet describes the cradle-to-gate production for C12-13 E2S Sodium Salt. C12-13 E2S is a petrochemical surfactant.

The ERASM SLE project recommends to use the data provided in a full ‘cradle-to-grave’ life cycle context of the surfactant in a real application.

Further information on the ERASM SLE project and the source of these datasets can be found in [2].

The full LCI can be accessed via www.erasm.org or via http://lcdn.thinkstep.com/Node/

Goal and Scope of ERASM SLE project [2]

The main goal was to update the existing LCI inventories [3,5,6] for the production of C12-13E2S and its main precursors/intermediates.

Temporal Coverage	Data collected represents a 12 month averages representing the year 2011, to compensate seasonal influence of data. Background data have reference years from 2008 to 2010. The dataset is considered to be valid until substantial technological changes in the production chain occur
Geographical Coverage	Data were based on five suppliers representing the C12-13 E2S (petro) production in Europe. The geographical representativeness for C12-13 E2S was considered ‘good’.
Technological Coverage	The technological representativeness for C12-13 E2S was considered ‘very good’. Figure 1 provides a schematic overview of the production process of C12-13 E2S.
Representativeness for market volume	>70% (Represented market volume (in mass) covered by primary data used in ERASM SLE project)
Declared Unit	In ERASM SLE project the declared unit (functional unit) and reference flow is one thousand kilogram (1000 kg) of surfactant active ingredient. This was the reference unit also used in [3]. Functional Unit: 1 metric tonne of C12-13 E2S (petro) 100% active substance.

<table>
<tr><td>Cradle-to Gate System Boundaries</td><td colspan="2">
<table>
<tr><th>Included</th><th>Excluded</th></tr>
<tr><td>Fatty alcohol C12-15 (petro) production (this production is further explained in the Eco Profile fact sheet of the precursor C12-15 fatty alcohol (#4))</td><td>Construction of major capital equipment (Infrastructure)</td></tr>
<tr><td>Sodium hydroxide and sulphur trioxide production</td><td>Maintenance and operation of support equipment</td></tr>
<tr><td>Energy production</td><td>Human labor and employee transport</td></tr>
<tr><td>Utilities</td><td>Packaging</td></tr>
<tr><td>Transportation processes for the main materials</td><td></td></tr>
<tr><td>Water use and treatment of waste water</td><td></td></tr>
<tr><td>Treatment of wastes</td><td></td></tr>
</table>
</td></tr>
<tr><td>Assumptions and Limitations</td><td colspan="2">Transportation was only considered for the main materials (covers about 90% of the mass of all inputs), other transportation was not considered.
Vehicle of transport for national transport were estimated as truck, where necessary.</td></tr>
<tr><td>Cut-off Criteria [4]</td><td colspan="2">No significant cut-offs were used.
The LCI study included all material inputs that had a cumulative total (refers to unit process level) of at least 98% of the total mass inputs to the unit process, and included all material inputs that had a cumulative total of at least 98% of total energy inputs to the unit process.
The study included any material that had environmental significance in its extraction, manufacture, use or disposal, is highly toxic, dangerous for the environment, or is classified as hazardous waste.
The sum of the excluded material flows did not exceed 5% of mass, energy or environmental relevance.</td></tr>
<tr><td rowspan="2">Calculation Rules</td><td>Allocation</td><td>For C12-13 E2S production allocation was not applied to the foreground system. However, allocation (mass/economic) was applied for some background data.</td></tr>
<tr><td>Aggregated data</td><td>Vertical averaging was considered (as long as the final product was the same, different processes with common product intermediates can be aggregated in the average)</td></tr>
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Life Cycle Inventory and Impact Assessment [2]

Based on the LCI data an environmental impact assessment was performed for the indicators Primary Energy Demand (PED) and Global Warming Potential (GWP). Other impacts may be calculated from the full LCI dataset.

Primary Energy Demand (PED): An analysis of the inventory data showed that the PED is significantly caused by the production of the petro based fatty alcohol (50% contribution) and its precursor ethylene oxide (30% of total). The production of sodium hydroxide accounts for about 5-10% of the PED. The generation of thermal energy, electricity and the production of other chemicals cause roughly less than 20% of total. The remaining 5% is due to transports, utilities, process waste treatment and direct emissions.

Global Warming Potential (GWP): An analysis of the inventory data showed that the GWP is mainly caused by the production of the precursor ethylene oxide (approx.25% of total) and the production of the petro based fatty alcohol (less than 50% contribution). The production of sodium hydroxide accounts for about 5-10% of the GWP. The generation of thermal energy, electricity and the production of other chemicals cause roughly less than 20% of total. The remaining (5% contribution) is due to transports, utilities, process waste treatment and direct emissions.
The small amount of carbon uptake is linked to the generation of electricity and transport fuels by the use of renewable energy carriers.

Table 1. Primary Energy Demand and air emissions related to Global Warming per 1 tonne of C12-13 E2S (petro) 100% active substance

LCI result	Unit	Amount
Primary energy demand		
Primary energy demand from renewable materials (net calorific value)	MJ	1602
Primary energy demand from fossil materials (net calorific value)	MJ	63441
Primary energy demand from fossil and renewable materials (net calorific value)	MJ	65043
Air emissions related to Global Warming Potential		
Carbon uptake, biotic	kg CO_2 equiv.	-77.8
Carbon dioxide, fossil	kg	2211
Carbon dioxide, biotic	kg	89
Carbon dioxide, from land use, land use change and peat oxidation	kg	0
Methane	kg	7.72
Nitrous oxide (laughing gas)	kg	0.04
NMVOC emissions	kg	1.83
*Total GWP (according to [**IPCC 2007**])*	*t CO_2-equiv.*	*2.43*

References for the ERASM SLE Project

Data Owner and Commissioner of the study	ERASM (Environment & Health Risk Assessment and Management). A research partnership of the Detergents and Surfactants Industries in Europe (www.erasm.org).
LCA Practitioner	thinkstep AG (www.thinkstep.com)
Reviewers	Prof. Walter Kloepffer, LCA Consult Mrs. Charlotte Petiot and Dr. Yannick Leguern, BioIS by Deloitte
References	[1] ECHA. http://echa.europa.eu [2] Schowanek. D *et al*. (2017) New and Updated Life Cycle Inventories for Surfactants used in European Detergents: Summary of the ERASM Surfactant Life Cycle and Ecofootprinting Project. Int J. LCA, in press. [3] CEFIC-Franklin (1994). Resource and environmental profile analysis of petrochemical and oleo chemical surfactants produced in Europe. Phase II Final Report, Franklin Associates, LTD [4] PLASTICSEUROPE (2011). Eco-profiles and Environmental Declarations – Life Cycle Inventory (LCI) Methodology and Product Category Rules (PCR) for Uncompounded Polymer Resins and Reactive Polymer Precursors, version 2.0. [5] Thomas, H. (1995). A life-cycle inventory for the production of alcohol ethoxy sulphates in Europe. Tenside Surf. Det. 32, 140-151. [6] Hirsinger, F. & Schick, K.-P. (1995). A life-cycle inventory for the production of alcohol sulfates in Europe. Tenside Surf. Det. 32, 128-139.

Figure1. Production process of C12-13 E2S (sodium salt).